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Asymptotic Study on the Extendability of Equilibria of Nematic Polymers

Hong Zhou

Department of Applied Mathematics
Naval Postgraduate School, Monterey, CA 93943, USA
hzhou@nps.edu

Hongyun Wang

Department of Applied Mathematics and Statistics
University of California, Santa Cruz, CA 95064, USA

Abstract

This paper addresses the extendability of equilibrium solutions of pure nematic liquid crystal polymers. More precisely, we apply the asymptotic analysis to show that the Jacobian of the nonlinear system is nonzero for both the prolate branch and the oblate branch when the nematic strength is large enough. This result implies the existence and uniqueness of the equilibrium solutions in the presence of small perturbations.

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1 Introduction

The kinetic Doi-Hess theory [6, 15] has been a useful tool for modeling nematic liquid crystal polymers (LCP). The Doi-Hess theory uses rigid rods to represent the nematogenic molecules and describe the ensemble with an orientational probability density function (pdf). The rotational transport equation for the orientational pdf is given by a nonlinear Smoluchowski (Fokker-Planck) equation. The Smoluchowski equation has attracted a lot of attentions from the mathematical society [2, 3, 4, 7, 8, 9, 10, 11, 12, 13, 14, 18, 19, 23, 21, 17, 24, 26, 22, 25].

In [24] we showed that for large values of the nematic strength and small perturbation there is a solution near the corresponding unperturbed pure nematic solution. The existence was established using complicated free energy arguments. Furthermore, only existence was established while the uniqueness was not shown. Here in this study we use the asymptotic analysis to show that for large values of the nematic strength, the Jacobian is nonzero. Therefore, we establish the extendability (both existence and uniqueness) of the equilibria of nematic polymers in the presence of small perturbations.

2 Nonlinear systems and equilibrium solutions

We briefly present the mathematical model system of the Doi-Hess kinetic theory for homogeneous flows of rigid rodlike nematogenic molecules immersed in a viscous solvent [6, 15]. By "homogeneous" it is meant that the LCP orientational distribution is uniform in space. We denote the orientational direction of each polymer rod by a unit vector $\mathbf{m}$. For pure nematic polymers, the total potential consists of only the Maier-Saupe interaction potential

$$U(\mathbf{m}) = -b\langle \mathbf{mm} \rangle : \mathbf{mm} \tag{1}$$

where the tensor product $\mathbf{mm}$ and tensor double contraction $\mathbf{A} : \mathbf{B}$ are defined as

$$\begin{aligned} \mathbf{mm} &\equiv \begin{pmatrix} m_1m_1 & m_1m_2 & m_1m_3 \\ m_2m_1 & m_2m_2 & m_2m_3 \\ m_3m_1 & m_3m_2 & m_3m_3 \end{pmatrix}, \\ \mathbf{A} : \mathbf{B} &\equiv \sum_{i,j} a_{ij}b_{ij}. \end{aligned} \tag{2}$$

In (1) $b = 3N/2$ and N is the normalized polymer concentration describing the strength of inter-molecular interactions, and $\langle\mathbf{mm}\rangle$ is the second moment of the orientation distribution:

$$\langle\mathbf{mm}\rangle \equiv \int_{||\mathbf{m}||=1} \mathbf{mm}\ \rho(\mathbf{m})\ d\mathbf{m}, \tag{3}$$

where $\rho(\mathbf{m}, t)$ is the orientational probability density function of the ensemble, i.e., the probability density that a polymer rod has direction $\mathbf{m}$ at time t. The potential (1) has been normalized with respect to k_BT where k_B is the Boltzmann constant and T the absolute temperature.

For pure nematic polymers, the equilibrium solutions of the Smoluchowski equation are described by the Boltzmann distribution [6]:

$$\rho(\mathbf{m}) = \frac{1}{Z}\exp[-U(\mathbf{m})], \tag{4}$$

where $Z = \int_S \exp[-U(\mathbf{m})]\, d\mathbf{m}$ is the partition function and S is the unit sphere.

Let us select the coordinate system such that the second moment $\langle\mathbf{mm}\rangle$ is diagonal:

$$\langle\mathbf{mm}\rangle = \begin{pmatrix} \langle m_1^2\rangle & 0 & 0 \\ 0 & \langle m_2^2\rangle & 0 \\ 0 & 0 & \langle m_3^2\rangle \end{pmatrix}. \tag{5}$$

As a consequence, the Maier-Saupe potential can be written as

$$U(\mathbf{m}) = -b(\langle m_1^2\rangle m_1^2 + \langle m_2^2\rangle m_2^2 + \langle m_3^2\rangle m_3^2). \tag{6}$$

The most significant conclusion for pure nematic polymers is that all equilibrium solutions are axisymmetric [7, 18, 23]. Since not all equilibrium solutions of a perturbed nematic polymer ensemble are axisymmetric, to facilitate the discussion of the extendability , we formulate the problem without using the axisymmetry. In the Boltzmann form (4), an equilibrium solution is completely specified by the second moment $\langle \mathbf{mm} \rangle$. Because of the constraint $m_1^2 + m_2^2 + m_3^2 = 1$, an equilibrium solution is completely specified by

$$s_1 \equiv \langle m_1^2 \rangle, \quad s_2 \equiv \langle m_2^2 \rangle. \tag{7}$$

We choose the coordinate system such that for nematic polymers without perturbation we have $s_1 = s_2$. In terms of (s_1, s_2), the Maier-Saupe potential can be expressed as

$$\begin{aligned} U(\mathbf{m}) &= -b(s_1\, m_1^2 + s_2\, m_2^2 + (1 - s_1 - s_2)\, m_3^2) \\ &= -b\left[\frac{1}{2}(s_2 - s_1)(m_2^2 - m_1^2) + (1 - \frac{3}{2}(s_1 + s_2))m_3^2\right] + const. \end{aligned} \tag{8}$$

From (7), the nonlinear system for (s_1, s_2) is

$$s_1 - \langle m_1^2 \rangle = 0, \quad s_2 - \langle m_2^2 \rangle = 0, \tag{9}$$

where the equilibrium pdf used in averaging is

$$\rho(\mathbf{m}) = \frac{1}{Z} \exp\left\{ b\left[\frac{1}{2}(s_2 - s_1)(m_2^2 - m_1^2) + (1 - \frac{3}{2}(s_1 + s_2))m_3^2\right]\right\}. \tag{10}$$

The form of the equilibrium pdf (10) suggests us to introduce a new pair of unknown variables

$$\eta_1 \equiv b\left[1 - \frac{3}{2}(s_1 + s_2)\right], \quad \eta_2 \equiv \frac{b}{2}(s_2 - s_1). \tag{11}$$

Or, equivalently, the nonlinear system for (η_1, η_2) is

$$\begin{aligned} F_1(\eta_1, \eta_2) &\equiv \frac{\eta_1}{b} - \frac{1}{2}(3\langle m_3^2 \rangle - 1) = 0, \\ F_2(\eta_1, \eta_2) &\equiv \frac{\eta_2}{b} - \frac{1}{2}\langle m_2^2 - m_1^2 \rangle = 0, \end{aligned} \tag{12}$$

where the equilibrium pdf used in averaging is

$$\rho(\mathbf{m}, \eta_1, \eta_2) = \frac{\exp\left[\eta_2(m_2^2 - m_1^2) + \eta_1 m_3^2\right]}{\int_S \exp\left[\eta_2(m_2^2 - m_1^2) + \eta_1 m_3^2\right]\, d\mathbf{m}}. \tag{13}$$

3 Jacobian of the nonlinear system

Recall that we have selected our coordinate system such that for pure nematic polymers we have $\eta_2 = 0$. Let us calculate the Jacobian of system (12) at an equilibrium of pure nematic polymer where $\eta_2 = 0$.

We start by finding the partial derivatives of pdf (13):

$$\begin{aligned}\frac{\partial}{\partial \eta_1}\rho(\mathbf{m},\eta_1,\eta_2) &= \frac{\partial}{\partial \eta_1}\frac{\exp\left[\eta_2(m_2^2-m_1^2)+\eta_1 m_3^2\right]}{\int_S \exp\left[\eta_2(m_2^2-m_1^2)+\eta_1 m_3^2\right]\, d\mathbf{m}} \\ &= (m_3^2 - \langle m_3^2\rangle)\rho(\mathbf{m},\eta_1,\eta_2), \qquad (14)\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial \eta_2}\rho(\mathbf{m},\eta_1,\eta_2) &= \frac{\partial}{\partial \eta_2}\frac{\exp\left[\eta_2(m_2^2-m_1^2)+\eta_1 m_3^2\right]}{\int_S \exp\left[\eta_2(m_2^2-m_1^2)+\eta_1 m_3^2\right]\, d\mathbf{m}} \\ &= (m_2^2 - m_1^2 - \langle m_2^2 - m_1^2\rangle)\rho(\mathbf{m},\eta_1,\eta_2). \qquad (15)\end{aligned}$$

Then the partial derivatives of (12) at an equilibrium ($\eta_1 = r, \eta_2 = 0$) are given by

$$\begin{aligned}\frac{\partial}{\partial \eta_1}F_1(\eta_1,\eta_2) &= \frac{1}{b} - \frac{3}{2}\langle m_3^2(m_3^2 - \langle m_3^2\rangle)\rangle = \frac{1}{b} - \frac{3}{2}\mathrm{var}(m_3^2), \\ \frac{\partial}{\partial \eta_2}F_1(\eta_1,\eta_2) &= -\frac{3}{2}\langle m_3^2(m_2^2 - m_1^2 - \langle m_2^2 - m_1^2\rangle)\rangle = 0, \qquad (16) \\ \frac{\partial}{\partial \eta_1}F_2(\eta_1,\eta_2) &= -\frac{1}{2}\langle (m_2^2 - m_1^2)(m_3^2 - \langle m_3^2\rangle)\rangle = 0, \\ \frac{\partial}{\partial \eta_2}F_2(\eta_1,\eta_2) &= \frac{1}{b} - \frac{1}{2}\langle (m_2^2 - m_1^2)(m_2^2 - m_1^2 - \langle m_2^2 - m_1^2\rangle)\rangle = \frac{1}{b} - \frac{1}{2}\langle (m_2^2 - m_1^2)^2\rangle.\end{aligned}$$

In the above calculations all averages are evaluated using the pdf

$$\rho(\mathbf{m},\eta_1 = r,\eta_2 = 0) = \frac{1}{Z}\exp(r m_3^2), \qquad (17)$$

where r satisfies the equation

$$\frac{r}{b} - \frac{1}{2}\left(3\langle m_3^2\rangle - 1\right) = 0. \qquad (18)$$

Now we write (18) in a more explicit form using spherical coordinates. We select the z-axis as the pole of the spherical coordinate system. The pdf (13) in spherical coordinates is of the form

$$\rho(\phi,\theta) = \frac{\exp(r\cos^2\phi)}{2\pi\int_0^\pi \exp(r\cos^2\phi)\,\sin\phi\, d\phi}. \qquad (19)$$

Substituting this expression into $3\langle m_3^2\rangle - 1$ yields

$$3\langle m_3^2\rangle - 1 = \frac{\int_0^\pi (3\cos^2\phi - 1)\exp(r\cos^2\phi)\,\sin\phi\,d\phi}{\int_0^\pi \exp(r\cos^2\phi)\,\sin\phi\,d\phi} = \frac{\int_0^1 (3u^2-1)\,\exp(ru^2)du}{\int_0^1 \exp(ru^2)\,du} \tag{20}$$

where a change of variable $u = \cos\phi$ is applied. Integrating by parts yields

$$3\langle m_3^2\rangle - 1 = \frac{\int_0^1 \exp(ru^2)d(u^3-u)}{\int_0^1 \exp(ru^2)\,du} = 2r\frac{\int_0^1 (u-u^3)u\exp(ru^2)du}{\int_0^1 \exp(ru^2)\,du}. \tag{21}$$

With the aid of (21), the equation (18) for r becomes

$$r\left[\frac{1}{b} - \frac{\int_0^1 u^2(1-u^2)\exp(ru^2)du}{\int_0^1 \exp(ru^2)\,du}\right] = 0. \tag{22}$$

Finally, it follows from (16) that the Jacobian of the nonlinear system (12) at an equilibrium is given by

$$\left.\frac{\partial(F_1,F_2)}{\partial(\eta_1,\eta_2)}\right|_{\substack{\eta_1=r\\ \eta_2=0}} = \left[\frac{1}{b} - \frac{3}{2}\mathrm{var}(m_3^2)\right]\cdot\left[\frac{1}{b} - \frac{1}{2}\langle(m_2^2-m_1^2)^2\rangle\right]. \tag{23}$$

We discuss several cases.

- <u>Case 1</u>: Equation (22) has a trivial solution $r = 0$, corresponding to the isotropic state. In the isotropic state,

$$\begin{aligned}
&\rho(\mathbf{m}) = \frac{1}{4\pi}, \quad \langle m_j^2\rangle = \frac{1}{3}, \quad \langle m_j^4\rangle = \frac{1}{5}, \quad \langle m_i^2 m_j^2\rangle = \frac{1}{15},\ i\neq j,\\
&\mathrm{var}(m_3^2) = \langle m_3^4\rangle - \langle m_3^2\rangle^2 = \frac{1}{5} - \frac{1}{9} = \frac{4}{45},\\
&\langle(m_2^2-m_1^2)^2\rangle = \langle m_2^4\rangle - 2\langle m_1^2 m_2^2\rangle + \langle m_1^4\rangle = \frac{2}{5} - \frac{2}{15} = \frac{4}{15}.
\end{aligned} \tag{24}$$

On substituting these results into the right-hand side of (23), we obtain

$$\begin{aligned}
&\frac{1}{b} - \frac{3}{2}\mathrm{var}(m_3^2) = \frac{1}{b} - \frac{2}{15} = 0 \text{ if and only if } b = \frac{15}{2},\\
&\frac{1}{b} - \frac{1}{2}\langle(m_2^2-m_1^2)^2\rangle = \frac{1}{b} - \frac{2}{15} = 0 \text{ if and only if } b = \frac{15}{2}.
\end{aligned} \tag{25}$$

It follows immediately that

$$\left.\frac{\partial(F_1,F_2)}{\partial(\eta_1,\eta_2)}\right|_{\substack{\eta_1=r\\ \eta_2=0}} = 0 \text{ if and only if } b = \frac{15}{2}. \tag{26}$$

Therefore, *away from $b = \frac{15}{2}$, the isotropic state can be extended.*

- Case 2: For $r \neq 0$, equation (22) is equivalent to

$$\frac{1}{b} = f(r), \text{ where } f(r) \equiv \frac{\int_0^1 u^2(1-u^2)\exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du}. \tag{27}$$

In [23] it has been shown that the function $f(r)$ has the following properties:

1. $f(0) = \frac{2}{15}$;
2. $\lim_{r\to+\infty} f(r) = 0$ and $\lim_{r\to-\infty} f(r) = 0$;
3. $f(r)$ attains its maximum at $r = r^* = 2.1782879748$ where $f(r^*) = 0.14855559992254$ and $b^* = \frac{1}{f(r^*)} = 6.7314863965$;
4. For $r < r^*$, $f(r)$ is strictly increasing; For $r > r^*$, $f(r)$ is strictly decreasing.

From the properties of the function $f(r)$, it is clear that equation (27) has a solution for $b < b^*$. For $b > b^*$, there are two solutions: $r_p(b) > r^*$ and $r_o(b) < r^*$. Here we use the subscript "p" to refer to a *prolate* state and the subscript "o" to refer to an *oblate* state even though this labeling is not completely precise. In fact, $r_p(b)$ corresponds to a prolate state for all values of $b > b^*$ while $r_o(b)$ corresponds to an oblate state only for $b > 7.5$. For $7.5 > b > b^*$, $r_o(b)$ corresponds to a prolate state. As $b \to +\infty$, we have

$$\lim_{b\to+\infty} r_p(b) = +\infty, \ \lim_{b\to+\infty} r_o(b) = -\infty. \tag{28}$$

Now we look at the asymptotic behaviors of the prolate branch ($r \to +\infty$) and the oblate branch ($r \to -\infty$). For mathematical convenience, we use r as the independent variable.

- **Case 2A: The prolate branch ($r \to +\infty$)**

Our approach is to expand $f(r)$ for $r \to +\infty$. First, to evaluate the integrals in (27), we make the change of variables:

$$v = 1 - u^2, \quad u = \sqrt{1-v},$$
$$dv = -2u\,du, \quad du = \frac{-1}{2\sqrt{1-v}}\,dv.$$

Substituting into the integrals in (27) yields

$$\int_0^1 \exp(ru^2)\,du = \int_0^1 \exp(r(1-v))\frac{1}{2\sqrt{1-v}}\,dv$$
$$= \frac{\exp(r)}{2}\int_0^1 \exp(-rv)(1+\frac{1}{2}v+\frac{3}{8}v^2+\cdots)\,dv$$
$$= \frac{\exp(r)}{2}\left(\frac{1}{r}+\frac{1}{2}\cdot\frac{1}{r^2}+\frac{3}{4}\cdot\frac{1}{r^3}+\cdots\right),$$

$$\int_0^1 u^2(1-u^2)\exp(ru^2)\,du = \int_0^1 (1-v)v\exp(r(1-v))\frac{1}{2\sqrt{1-v}}\,dv$$
$$= \frac{\exp(r)}{2}\int_0^1 \exp(-rv)(1-v)v\left(1+\frac{1}{2}v+\frac{3}{8}v^2+\cdots\right)\,dv$$
$$= \frac{\exp(r)}{2}\int_0^1 \exp(-rv)\left(v-\frac{1}{2}v^2-\frac{1}{8}v^3+\cdots\right)\,dv$$
$$= \frac{\exp(r)}{2}\left(\frac{1}{r^2}-\frac{1}{r^3}-\frac{3}{4}\cdot\frac{1}{r^4}+\cdots\right).$$

By using these asymptotic results, equation (27) can now be written as

$$\frac{1}{b} = f(r) = \frac{\int_0^1 u^2(1-u^2)\exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du} = \frac{\frac{1}{r^2}\left(1-\frac{1}{r}-\frac{3}{4}\cdot\frac{1}{r^2}+\cdots\right)}{\frac{1}{r}\left(1+\frac{1}{2}\cdot\frac{1}{r}+\frac{3}{4}\cdot\frac{1}{r^2}+\cdots\right)}$$
$$= \frac{1}{r}\left(1-\frac{3}{2}\cdot\frac{1}{r}-\frac{3}{4}\frac{1}{r^2}+\cdots\right).$$

The order parameter is given by

$$\frac{1}{2}(3\langle m_3^2\rangle - 1) = \frac{r}{b} = 1-\frac{3}{2}\cdot\frac{1}{r}-\frac{3}{4}\cdot\frac{1}{r^2}+\cdots.$$

Now we calculate $\mathrm{var}(m_3^2)$ and $\langle(m_2^2-m_1^2)^2\rangle$. We note that

$$\mathrm{var}(m_3^2) = \mathrm{var}(1-m_3^2) = \langle(1-m_3^2)^2\rangle - \langle 1-m_3^2\rangle^2.$$

Introducing change of variable $u=\cos\phi$, we get

$$\langle 1-m_3^2\rangle = \frac{\int_0^\pi \sin^2\phi\,\exp(r\cos^2\phi)\,\sin\phi\,d\phi}{\int_0^\pi \exp(r\cos^2\phi)\,\sin\phi\,d\phi} = \frac{\int_0^1 (1-u^2)\,\exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du},$$

$$\langle(1-m_3^2)^2\rangle = \frac{\int_0^\pi \sin^4\phi\,\exp(r\cos^2\phi)\,\sin\phi\,d\phi}{\int_0^\pi \exp(r\cos^2\phi)\,\sin\phi\,d\phi} = \frac{\int_0^1 (1-u^2)^2\,\exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du}, \qquad (29)$$

$$\langle(m_2^2-m_1^2)^2\rangle = \frac{\frac{1}{2}\int_0^\pi \sin^4\phi\,\exp(r\cos^2\phi)\,\sin\phi\,d\phi}{\int_0^\pi \exp(r\cos^2\phi)\,\sin\phi\,d\phi} = \frac{1}{2}\frac{\int_0^1 (1-u^2)^2\,\exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du}.$$

Note that

$$\int_0^1 (1-u^2)\ \exp(ru^2)\,du = \int_0^1 v\ \exp(r(1-v))\,\frac{1}{2\sqrt{1-v}}\,dv$$

$$= \frac{\exp(r)}{2}\int_0^1 \exp(-rv)(v+\frac{1}{2}v^2+\cdots)\,dv = \frac{\exp(r)}{2}(\frac{1}{r^2}+\frac{1}{r^3}+\cdots), \tag{30}$$

$$\int_0^1 (1-u^2)^2\ \exp(ru^2)\,du = \int_0^1 v^2\exp(r(1-v))\frac{1}{2\sqrt{1-v}}\,dv$$

$$= \frac{\exp(r)}{2}\int_0^1 \exp(-rv)(v^2+\frac{1}{2}v^3+\cdots)\,dv = \frac{\exp(r)}{2}(\frac{2}{r^3}+\frac{3}{r^4}+\cdots).$$

Substitution of (30) into (29) leads to

$$\langle 1-m_3^2\rangle = \frac{\int_0^1(1-u^2)\ \exp(ru^2)\,du}{\int_0^1\exp(ru^2)\,du} = \frac{\frac{1}{r^2}(1+\frac{1}{r}+\cdots)}{\frac{1}{r}(1+\frac{1}{2}\cdot\frac{1}{r}+\cdots)}$$

$$= \frac{1}{r}(1+\frac{1}{2}\cdot\frac{1}{r}+\cdots),$$

$$\langle(1-m_3^2)^2\rangle = \frac{\int_0^1(1-u^2)^2\ \exp(ru^2)\,du}{\int_0^1\exp(ru^2)\,du} = \frac{\frac{2}{r^3}(1+\frac{3}{2}\cdot\frac{1}{r}+\cdots)}{\frac{1}{r}(1+\frac{1}{2}\cdot\frac{1}{r}+\cdots)}$$

$$= \frac{2}{r^2}(1+\frac{1}{r}+\cdots),$$

$$\langle(m_2^2-m_1^2)^2\rangle = \frac{1}{2}\frac{\int_0^1(1-u^2)^2\ \exp(ru^2)\,du}{\int_0^1\exp(ru^2)\,du} = \frac{\frac{1}{r^3}(1+\frac{3}{2}\cdot\frac{1}{r}+\cdots)}{\frac{1}{r}(1+\frac{1}{2}\cdot\frac{1}{r}+\cdots)}$$

$$= \frac{1}{r^2}(1+\frac{1}{r}+\cdots).$$

Hence

$$\frac{1}{b}-\frac{3}{2}\mathrm{var}(m_3^2) = \frac{1}{b}-\frac{3}{2}\left(\langle(1-m_3^2)^2\rangle - \langle 1-m_3^2\rangle^2\right)$$

$$= \frac{1}{r}(1-\frac{3}{2}\cdot\frac{1}{r}-\frac{3}{4}\frac{1}{r^2}+\cdots) - \frac{3}{2}\left[\frac{2}{r^2}(1+\frac{1}{r}+\cdots)-\frac{1}{r^2}(1+\frac{1}{2}\cdot\frac{1}{r}+\cdots)^2\right]$$

$$= \frac{1}{r}(1-\frac{3}{2}\cdot\frac{1}{r}-\frac{3}{4}\frac{1}{r^2}+\cdots) - \frac{3}{2}\cdot\frac{1}{r^2}(1+\frac{1}{r}+\cdots)$$

$$= \frac{1}{r}(1 - 3 \cdot \frac{1}{r} - \frac{9}{4} \cdot \frac{1}{r^2} + \cdots) > 0 \text{ for large } r,$$

$$\frac{1}{b} - \frac{1}{2}\langle (m_2^2 - m_1^2)^2 \rangle = \frac{1}{r}(1 - \frac{3}{2} \cdot \frac{1}{r} - \frac{3}{4}\frac{1}{r^2} + \cdots) - \frac{1}{2} \cdot \frac{1}{r^2}(1 + \frac{1}{r} + \cdots)$$

$$= \frac{1}{r}(1 - 2 \cdot \frac{1}{r} - \frac{5}{4} \cdot \frac{1}{r^2} + \cdots) > 0 \text{ for large } r. \tag{31}$$

Consequently, it follows from (23) that

$$\left. \frac{\partial(F_1, F_2)}{\partial(\eta_1, \eta_2)} \right|_{\substack{\eta_1 = r \\ \eta_2 = 0}} > 0 \text{ for large } r.$$

Therefore, *for large r (large b), the prolate branch is extendable.*

- **Case 2B: The oblate branch ($r \to -\infty$)**

We use the same approach as before where the key step is to expand $f(r)$ for $\lambda = -r \to +\infty$. To do so, we introduce the change of variables

$$\begin{aligned} & v = u^2, \quad u = \sqrt{v}, \\ & dv = 2u\, du, \quad du = \frac{1}{2\sqrt{v}}\, dv. \end{aligned}$$

Then the integrals in (27) turn into

$$\int_0^1 \exp(ru^2)\, du = \int_0^1 \exp(-\lambda\, v) \frac{1}{2\sqrt{v}}\, dv$$

$$= \frac{1}{2} \cdot \frac{\Gamma(\frac{1}{2})}{\sqrt{\lambda}} = \frac{\sqrt{\pi}}{2} \cdot \frac{1}{\sqrt{-r}},$$

$$\int_0^1 u^2(1-u^2)\exp(ru^2)\, du = \int_0^1 (1-v)v \exp(r(1-v)) \frac{1}{2\sqrt{1-v}}\, dv$$

$$= \int_0^1 (1-v)v \exp(-\lambda v)\, \frac{1}{2\sqrt{v}}\, dv$$

$$= \frac{1}{2} \int_0^1 \exp(-\lambda v) \left(\sqrt{v} - v^{\frac{3}{2}}\right)\, dv$$

$$= \frac{1}{2}\left(\frac{\Gamma(\frac{3}{2})}{\lambda^{3/2}} - \frac{\Gamma(\frac{5}{2})}{\lambda^{5/2}}\right) = \frac{\sqrt{\pi}}{2}\left(\frac{1}{2} \cdot \frac{1}{(-r)^{3/2}} - \frac{3}{4} \cdot \frac{1}{(-r)^{5/2}}\right).$$

With the help of these results, (27) can be rewritten as

$$\frac{1}{b} = f(r) = \frac{\int_0^1 u^2(1-u^2)\exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du} = \frac{\frac{1}{\sqrt{-r}}\cdot\frac{1}{(-r)}\left[\frac{1}{2}-\frac{3}{4}\cdot\frac{1}{(-r)}\right]}{\frac{1}{\sqrt{-r}}}$$

$$= \frac{1}{(-r)}\left[\frac{1}{2}-\frac{3}{4}\cdot\frac{1}{(-r)}\right]. \tag{32}$$

The order parameter is given by

$$\frac{1}{2}(3\langle m_3^2\rangle - 1) = \frac{r}{b} = -\frac{1}{2}+\frac{3}{4}\cdot\frac{1}{(-r)}.$$

In order to calculate $\mathrm{var}(m_3^2)$ and $\langle (m_2^2-m_1^2)^2\rangle$. we observe that

$$\langle m_3^4\rangle = \frac{\int_0^\pi \cos^4\phi\ \exp(r\cos^2\phi)\ \sin\phi\,d\phi}{\int_0^\pi \exp(r\cos^2\phi)\ \sin\phi\,d\phi}$$

$$= \frac{\int_0^1 u^4\ \exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du} = \frac{\int_0^1 v^2\exp(rv)\frac{1}{2\sqrt{v}}\,dv}{\frac{\sqrt{\pi}}{2}\cdot\frac{1}{\sqrt{-r}}}$$

$$= \frac{\frac{1}{2}\Gamma(\frac{5}{2})\cdot(-r)^{-\frac{5}{2}}}{\frac{\sqrt{\pi}}{2}\cdot\frac{1}{\sqrt{-r}}} = \frac{3}{4r^2},$$

and

$$\langle m_3^2\rangle = \frac{\int_0^\pi \cos^2\phi\ \exp(r\cos^2\phi)\ \sin\phi\,d\phi}{\int_0^\pi \exp(r\cos^2\phi)\ \sin\phi\,d\phi}$$

$$= \frac{\int_0^1 u^2\ \exp(ru^2)\,du}{\int_0^1 \exp(ru^2)\,du} = \frac{\int_0^1 v\exp(rv)\frac{1}{2\sqrt{v}}\,dv}{\frac{\sqrt{\pi}}{2}\cdot\frac{1}{\sqrt{-r}}}$$

$$= \frac{\frac{1}{2}\Gamma(\frac{3}{2})\cdot(-r)^{-\frac{3}{2}}}{\frac{\sqrt{\pi}}{2}\cdot\frac{1}{\sqrt{-r}}} = -\frac{1}{2r}.$$

So we have

$$\mathrm{var}(m_3^2) = \langle m_3^4\rangle - \langle m_3^2\rangle^2 = \frac{3}{4r^2} - (-\frac{1}{2r})^2 = \frac{1}{2r^2},$$

$$\langle (m_2^2-m_1^2)^2\rangle = \frac{1}{2}\cdot\frac{\int_0^1(1-u^2)^2\exp(ru^2)\,du}{\int_0^1\exp(ru^2)\,du}$$

$$= \frac{1}{2} \cdot \frac{\frac{\sqrt{\pi}}{2}\left(\frac{1}{(-r)^{1/2}} - \frac{1}{(-r)^{3/2}} + \cdots\right)}{\frac{\sqrt{\pi}}{2} \cdot \frac{1}{\sqrt{-r}}} = \frac{1}{2} - \frac{1}{2(-r)} + \cdots. \tag{33}$$

Collecting all the above results, we find

$$\frac{1}{b} - \frac{3}{2}\mathrm{var}(m_3^2) = \frac{1}{(-r)}\left[\frac{1}{2} - \frac{3}{4} \cdot \frac{1}{(-r)}\right] - \frac{3}{2} \cdot \frac{1}{2r^2}$$

$$= -\frac{1}{2r} - \frac{3}{2r^2} > 0 \ \text{ as } r \to -\infty,$$

$$\frac{1}{b} - \frac{1}{2}\langle (m_2^2 - m_1^2)^2 \rangle = \frac{1}{(-r)}\left[\frac{1}{2} - \frac{3}{4}\frac{1}{(-r)}\right] - \frac{1}{2}\left(\frac{1}{2} - \frac{1}{2(-r)} + \cdots\right)$$

$$= -\frac{1}{4} + \frac{3}{4(-r)} + \cdots < 0 \ \text{ as } r \to -\infty. \tag{34}$$

Thus, from (23) we arrive at

$$\left.\frac{\partial(F_1, F_2)}{\partial(\eta_1, \eta_2)}\right|_{\substack{\eta_1 = r \\ \eta_2 = 0}} < 0 \ \text{ as } r \to -\infty.$$

In summary, *the oblate branch is extendable as* $r \to -\infty$.

4 Conclusions

We have applied the asymptotic analysis to show that the equilibrium solutions of the pure nematic polymers are extendable for large values of b where b is the nematic strength.

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References

[1] B. Bird, R. C. Armstrong and O. Hassager, *Dynamics of Polymeric Liquids*, vol. 1, Wiley, 1987.

[2] P. Constantin, I. Kevrekidis, and E. S. Titi, Asymptotic states of a Smoluchowski equation, Arch. Rat. Mech. Anal. 174 (2004), 365-384.

[3] P. Constantin, I. Kevrekidis, and E.S. Titi, Remarks on a Smoluchowski equation, Discrete and Continuous Dynamical Systems 11 (2004), 101-112.

[4] P. Constantin and J. Vukadinovic, Note on the number of steady states for a 2D Smoluchowski equation, Nonlinearity 18 (2005), 441-443.

[5] A. M. Donald, A. H. Windle and S. Hanna, *Liquid crystalline polymers*, Cambridge University Press, 2nd edition, 2006.

[6] M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Oxford University Press, 1986.

[7] I. Fatkullin and V. Slastikov, Critical points of the Onsager functional on a sphere, Nonlinearity 18 (2005), 2565-2580.

[8] M. G. Forest, R. Zhou and Q. Wang, Symmetries of the Doi kinetic theory for nematic polymers of arbitrary aspect ratio: at rest and in linear flows, Phys. Rev. E 66 (2002), 031712.

[9] M. G. Forest, Q. Wang and R. Zhou, The flow-phase diagram of Doi-Hess theory for sheared nematic polymers II: finite shear rates, Rheol. Acta 44(1) (2004), 80-93.

[10] M. G. Forest, R. Zhou and Q. Wang, The weak shear phase diagram for nematic polymers, Rheol. Acta 43(1) (2004), 17-37.

[11] M. G. Forest, R. Zhou and Q. Wang, Chaotic boundaries of nematic polymers in mixed shear and extensional flows, Physical Review Letters 93(8) (2004), 088301-088305.

[12] M. G. Forest, R. Zhou and Q. Wang, Kinetic structure simulations of nematic polymers in plane Couette cells, I: The algorithm and benchmarks, SIAM MMS 3(4) (2005), 853-870.

[13] M. G. Forest, R. Zhou and Q. Wang, Scaling behavior of kinetic orientational distributions for dilute nematic polymers in weak shear, J. Non-Newtonian Fluid Mech. 116 (2004), 183-204.

[14] M. G. Forest, and Q. Wang, Monodomain response of finite-aspect-ratio macromolecules in shear and related linear flows, Rheol. Acta 42 (2003), 20-46.

[15] S.Z. Hess, Fokker-Planck-equation approach to flow alignment in liquid crystals, Z. Naturforsch. A 31A (1976), 1034-1037.

[16] S. Hess and M. Kroger, Regular and chaotic orientational and rheological behaviour of liquid crystals, J. Phys.: Condens. Matter 16 (2004), S3835-S3859.

[17] G. Ji, Q. Wang, P. Zhang and H. Zhou, Study of phase transition in homogeneous, rigid extended nematics and magnetic suspensions using an order-reduction method, Physics of Fluid 18 (2006), 123103.

[18] H. Liu, H. Zhang and P. Zhang, Axial symmetry and classification of stationary solutions of Doi-Onsager equation on the sphere with Maier-Saupe potential, Comm. Math. Sci. 3 (2005), 201-218.

[19] C. Luo, H. Zhang and P. Zhang, The structure of equilibrium solution of 1D Smoluchowski equation, Nonlinearity 18 (2005), 379-389.

[20] A.D. Rey and M.M. Denn, Dynamical phenomena in liquid-crystalline materials, Annual Review of Fluid Mechanics, 34 (2002), 233-266.

[21] Q. Wang, S. Sircar and H. Zhou, Steady state solutions of the Smoluchowski equation for rigid nematic polymers under imposed fields, Comm. Math. Sci. 3 (2005), 605-620.

[22] A. Zarnescu, The stationary 2D Smoluchowski equation in strong homogeneous flow, Nonlinearity 19 (2006), 1619-1628.

[23] H. Zhou, H. Wang, M. G. Forest and Q. Wang, A new proof on axisymmetric equilibria of a three-dimensional Smoluchowski equation, Nonlinearity 18 (2005), 2815-2825.

[24] H. Zhou, H. Wang, Q. Wang, and M. G. Forest, Characterization of stable kinetic equilibria of rigid, dipolar rod ensembles for coupled dipole-dipole and Maier-Saupe potentials, Nonlinearity 20 (2007), 277-297.

[25] H. Zhou and H. Wang, Steady states and dynamics of 2-D nematic polymers driven by an imposed weak shear, Comm. Math. Sci. 5 (2007), 113-132.

[26] H. Zhou, H. Wang, and Q. Wang, Nonparallel solutions of extended nematic polymers under an external field, Discrete and Continuous Dynamical Systems-Series B, 7(4) (2007), 907-929.

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